Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supplementary material

"Importance of the decoration in shaped cobalt nanoparticles in the acceptor-less secondary alcohol dehydrogenation"

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1. Syntheses protocols

1.1. *Materials*

$Co(CH_3CO_2)_2 \cdot 4H_2O$ (Aldrich, > 98 %), $CoCl_2 \cdot 6H_2O$ (Alfa Aesar, 98%), $RuCl_3 \cdot xH_2O$ (Aldrich, 99.98 % or Sigma Aldrich, 38.0-42.0% Ru basis), $RuCl_3$ (Aldrich, Ru Content 45-55%), NaOH (Acros, micropearls or Sigma Aldrich, ≥97%), 1,2-butanediol (Fluka, 98% or Sigma Aldrich, ≥98%), 1,2-propanediol (Acros, 99%), lauric (Alfa Aesar, 98%), palmitic (Alfa Aesar, 95%), heptanoic (Aldrich, ≥ 99%), octanoic (Aldrich, ≥ 98%) and decanoic (Alfa Aesar, 99%) acids, methanol (MeOH, Sigma Aldrich, ≥99.8%) and ethanol (EtOH, Sigma Aldrich, ≥99.5%) were used as received. 2-octanol (Alfa Aesar, 98%), 2-octanone (Aldrich, 99.5%), n-decane (Carl Roth, 99%) were used as received in the catalytic tests.

1.2. *Preparation of cobalt precursors*

Home-made cobalt carboxylates, $Co(C_nH_{2n+1}CO_2)_2$ ($n = 6\text{-}15$), were used for the following nanoparticles syntheses.

- Synthesis of $Co(C_nH_{2n+1}CO_2)_2$, $n = 6, 7, 9$

In a 1 L beaker, NaOH (168 mmol) and the long-chain carboxylic acid (176 mmol) were dissolved in 160 mL of distilled water and the mixture was heated to 60°C for 30 min under mechanical stirring to yield a transparent solution. To this solution was then added dropwise under vigorous stirring (200 rpm) an aqueous solution (40 mL) of Co(II) acetate (80 mmol) preheated at 60°C for 15 min. This resulted in the formation of a pink precipitate which was left under stirring for 30 min at the same temperature. The solid was recovered by centrifugation (8500 rpm, 15 min), washed three times with distilled water (200 mL) and dried in an oven at 50°C for three days.

- $Co(C_nH_{2n+1}CO_2)_2$, $n = 11, 15$

First, 360 mmol lauric acid (L), respectively palmitic acid (P), and 360 mmol of sodium hydroxide were added in distilled water (300 mL) and heated at 80°C for 30 min under magnetic stirring to get a clear solution of NaL, respectively NaPa. The solutions were cooled down at room temperature. Then, an aqueous solution containing 180 mmol of $CoCl_2 \cdot 6H_2O$ was added slowly into the former solution under vigorous stirring using an Ultra-Turax homogenizer. The suspension was stirred for 30 min to obtain a pink powder of cobalt laurate, respectively cobalt palmitate, floating on the water solution. The pink powders were isolated using Buchner Funnel Filtration Process.

Several phases were obtained depending on the drying procedure. The di-hydrate cobalt laurate $Co(C_{11}H_{23}CO_2)_2{\cdot}2H_2O$ and cobalt palmitate $Co(C_{15}H_{31}CO_2)_2{\cdot}2\ H_2O$, hereafter called L1 and P1, respectively, were obtained after a drying at 50°C for 20 h. The anhydrous cobalt laurate called L2 was obtained drying the compound L1 at 50°C for 3 days. The anhydrous cobalt laurate called L3 was obtained drying the compound L1 at 50°C for 7 days. The anhydrous cobalt laurate called L4 was obtained drying the compound L1 at 100°C for 30 minutes. The anhydrous cobalt palmitate called P2 was obtained by drying the compound P1 at 65°C for 22 h. The anhydrous cobalt palmitate, called P3, was obtained drying the compound P1 at 85°C for 15 hours. The anhydrous cobalt palmitate called P4 was obtained drying the compound P1 at 100°C for 30 minutes.

1.3. Preparation of the Co NPs

- *Rods*

Samples H-R, O-R and D-R

To 100 mL of 1,2-butanediol, were added: the cobalt (II) carboxylate precursor (80 mM), $RuCl_3{\cdot}xH_2O$ ([Ru]/[Ru+Co] = 2.5 mol%) and sodium hydroxide (75 mM). The mixture was then heated under stirring at 100 rpm to 175°C with a heating rate of 8 °C min^{-1} for half an hour until the color of the solution turned black, indicating the reduction of Co(II) into metallic cobalt. After cooling down to room temperature, the cobalt particles were recovered using a permanent magnet, washed four times with 50 mL of absolute ethanol, and finally dried overnight in an oven at 50°C. Samples prepared using heptanoate, octanoate and decanoate capping agents were labelled H-R, O-R and D-R, respectively.

Sample L-R-1

To 1 L of 1,2-butanediol, were added: the cobalt (II) laurate called L2 (80 mM), $RuCl_3{\cdot}xH_2O$ ([Ru]/[Ru+Co] = 2.5 mol%) and sodium hydroxide (75 mM). The mixture was then heated under stirring at 100 rpm to 175°C with a heating rate of 8 °C min^{-1} for half an hour until the color of the solution turned black, indicating the reduction of Co(II) into metallic cobalt. After cooling down to room temperature, the cobalt particles were recovered using a permanent magnet, washed four times with 100 mL of absolute ethanol, and finally dried overnight in an oven at 50°C.

Sample L-R-2

To 1 L of 1,2-butanediol, were added: the cobalt (II) laurate called L1 (80 mM), $RuCl_3 \cdot xH_2O$ ([Ru]/[Ru+Co] = 2.5 mol%) and sodium hydroxide (75 mM). The mixture was then heated under stirring at 100 rpm to 175°C with a heating rate of 8 °C min^{-1} for half an hour until the color of the solution turned black, indicating the reduction of Co(II) into metallic cobalt. After cooling down to room temperature, the cobalt particles were recovered using a permanent magnet, washed four times with 100 mL absolute ethanol, and finally dried overnight in an oven at 50°C.

Sample L-R-3

To 100 mL of 1,2-butanediol, were added: the cobalt (II) laurate called L4 (80 mM), anhydrous $RuCl_3$ ([Ru]/[Ru+Co] = 2.5 mol%) and sodium laurate (160 mM). The mixture was then heated under stirring at 100 rpm to 175°C with a heating rate of 8 °C min^{-1} for half an hour until the color of the solution turned black, indicating the reduction of Co(II) into metallic cobalt. After cooling down to room temperature, the cobalt particles were recovered using a permanent magnet, washed three times with 100 mL of absolute ethanol, and finally dried overnight in an oven at 50°C.

Sample L-R-4

To 100 mL of 1,2-butanediol, were added: the cobalt (II) laurate called L3 (80 mM), $RuCl_3 \cdot xH_2O$ ([Ru]/[Ru+Co] = 2.5 mol%) and sodium hydroxide (75 mM). The mixture was then heated under stirring at 100 rpm to 175°C with a heating rate of 8 °C min^{-1} for half an hour until the color of the solution turned black, indicating the reduction of Co(II) into metallic cobalt. After cooling down to room temperature, the cobalt particles were recovered using a permanent magnet, washed three times with 100 mL of absolute ethanol, and finally dried overnight in an oven at 50°C.

Sample P-R-1

To 100 mL of 1,2-butanediol, were added: the cobalt (II) palmitate called P4 (80 mM), $RuCl_3 \cdot xH_2O$ ([Ru]/[Ru+Co] = 2.5 mol%) and sodium hydroxide (75 mM). The mixture was then heated under stirring at 100 rpm to 175°C with a heating rate of 8 °C min^{-1} for half an hour until the color of the solution turned black, indicating the reduction of Co(II) into metallic cobalt. After cooling down to room temperature, the cobalt particles were recovered using a permanent magnet, washed three times with 100 mL of absolute ethanol, and finally dried overnight in an oven at 50°C.

Sample P-R-2

To 100 mL of 1,2-butanediol, were added: the cobalt (II) palmitate called P2 (80 mM), $RuCl_3 \cdot xH_2O$ ([Ru]/[Ru+Co] = 2.5 mol%) and sodium hydroxide (75 mM). The mixture was then heated under stirring at 100 rpm to 175°C with a heating rate of 8 $°C\ min^{-1}$ for half an hour until the color of the solution turned black, indicating the reduction of Co(II) into metallic cobalt. After cooling down to room temperature, the cobalt particles were recovered using a permanent magnet, washed three times with 100 mL of absolute ethanol, and finally dried overnight in an oven at 50°C.

Sample P-R-3

To 100 mL of 1,2-butanediol, were added: the cobalt (II) palmitate called P4 (80 mM), anhydrous $RuCl_3$ ([Ru]/[Ru+Co] = 2.5 mol%) and sodium hydroxide (75 mM). The mixture was then heated under stirring at 100 rpm to 175°C with a heating rate of 8 $°C\ min^{-1}$ for half an hour until the color of the solution turned black, indicating the reduction of Co(II) into metallic cobalt. After cooling down to room temperature, the cobalt particles were recovered using a permanent magnet, washed three times with 100 mL of absolute ethanol, and finally dried overnight in an oven at 50°C.

- *Diabolos*

Sample L-D

To 100 mL of 1,2-propanediol, were added: the cobalt (II) laurate called L4 (80 mM), anhydrous $RuCl_3$ ([Ru]/[Ru+Co] = 2.5 mol%) and sodium hydroxide (75 mM). The mixture was then heated under stirring at 100 rpm to 175°C with a heating rate of 8 $°C\ min^{-1}$ for half an hour until the color of the solution turned black, indicating the reduction of Co(II) into metallic cobalt. After cooling down to room temperature, the cobalt particles were recovered using a permanent magnet, washed three times with 100 mL of absolute ethanol, and finally dried overnight in an oven at 50°C.

Sample P-D

To 100 mL of 1,2-butanediol, were added: the cobalt (II) palmitate called P4 (80 mM), anhydrous $RuCl_3$ ([Ru]/[Ru+Co] = 2.5 mol%) and sodium palmitate (160 mM). The mixture was then heated under stirring at 100 rpm to 175°C with a heating rate of 8 $°C \cdot min^{-1}$ for half an hour until the color of the solution turned black, indicating the reduction of Co(II) into metallic cobalt. After cooling down to room temperature, the cobalt particles were recovered using a permanent magnet, washed six times with 100 mL of methanol, and finally dried overnight in an oven at 50°C.

- *Platelets*

Sample L-P

To 100 mL of 1,2-propanediol, were added: the cobalt (II) laurate called L4 (80 mM), anhydrous $RuCl_3$ ([Ru]/[Ru+Co] = 2.5 mol%) and sodium laurate (160 mM). The mixture was then heated under stirring at 100 rpm to 175°C with a heating rate of 8 °C min^{-1} for half an hour until the color of the solution turned black, indicating the reduction of Co(II) into metallic cobalt. After cooling down to room temperature, the cobalt particles were recovered using a permanent magnet, washed three times with 120 mL of absolute ethanol, and finally dried overnight in an oven at 50°C.

Sample P-P

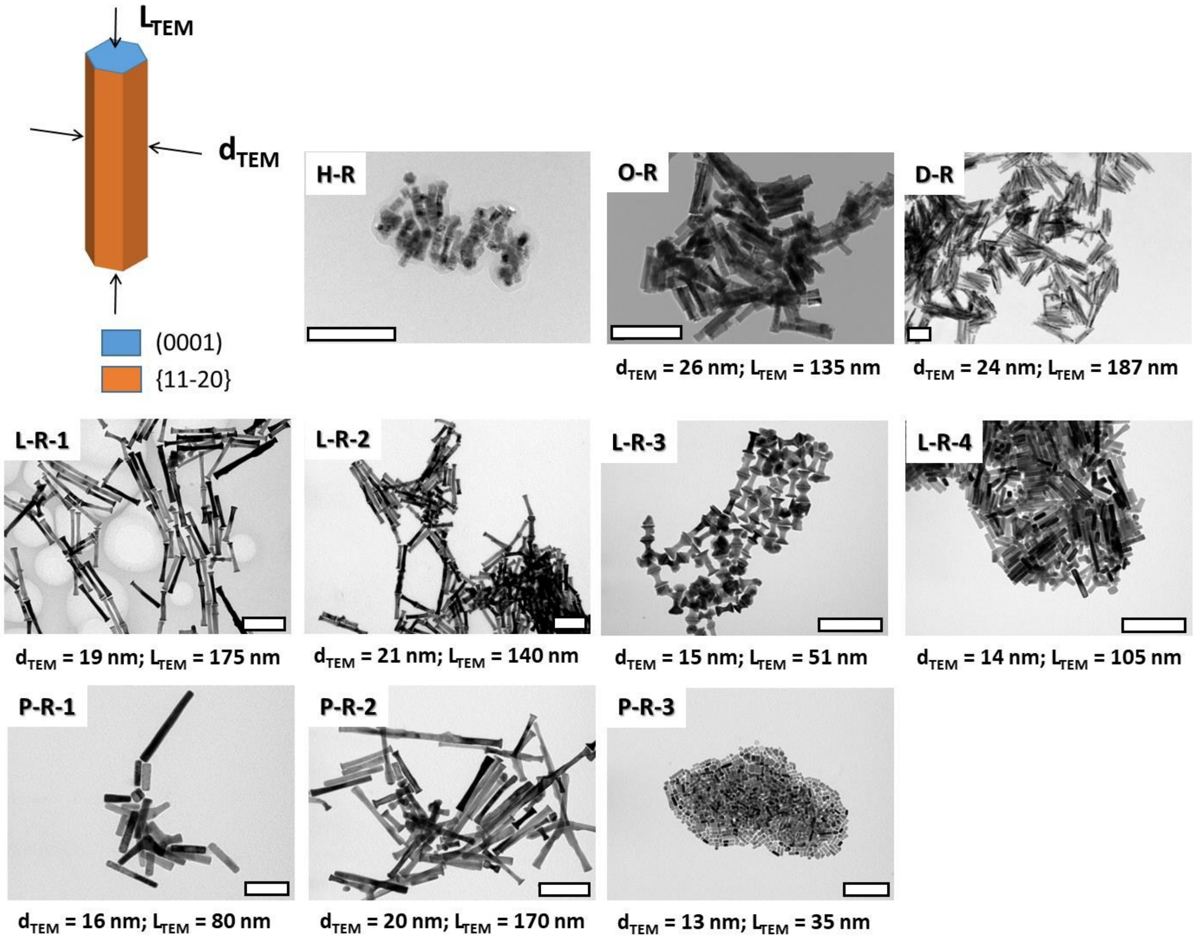
To 100 mL of 1,2-propanediol, were added: the cobalt (II) palmitate called P4 (80 mM), anhydrous $RuCl_3$ ([Ru]/[Ru+Co] = 2.5 mol%) and sodium palmitate (160 mM). The mixture was then heated under stirring at 100 rpm to 175°C with a heating rate of 8 °C min^{-1} for half an hour until the color of the solution turned black, indicating the reduction of Co(II) into metallic cobalt. After cooling down to room temperature, the cobalt particles were recovered using a permanent magnet, washed three times with 120 mL of absolute ethanol, and finally dried overnight in an oven at 50°C.

1.4. Summary of the experimental conditions for the synthesis of the different cobalt samples

Sample	Cobalt precursor	Nucleating Agent	Base	Polyol
L-R-1	Cobalt laurate “L2”	$RuCl_3{\cdot}xH_2O$	Sodium hydroxide 0.075 M	1,2-butanediol
L-R-2	Cobalt laurate “L1”	$RuCl_3{\cdot}xH_2O$	Sodium hydroxide 0.075 M	1,2-butanediol
L-R-3	Cobalt laurate “L4”	anhydrous $RuCl_3$	Sodium laurate 0.16 M	1,2-butanediol
L-R-4	Cobalt laurate “L3”	$RuCl_3{\cdot}xH_2O$	Sodium hydroxide 0.075 M	1,2-butanediol
L-D	Cobalt laurate “L4”	anhydrous $RuCl_3$	Sodium hydroxide 0.075 M	1,2-propanediol
L-P	Cobalt laurate “L4”	anhydrous $RuCl_3$	Sodium laurate 0.16 M	1,2-propanediol
P-R-1	Cobalt palmitate “P4”	$RuCl_3{\cdot}xH_2O$	Sodium hydroxide 0.075 M	1,2-butanediol
P-R-2	Cobalt palmitate “P2”	$RuCl_3{\cdot}xH_2O$	Sodium hydroxide 0.075 M	1,2-butanediol
P-R-3	Cobalt palmitate “P4”	anhydrous $RuCl_3$	Sodium hydroxide 0.075 M	1,2-butanediol
P-D	Cobalt palmitate “P4”	anhydrous $RuCl_3$	Sodium palmitate 0.16 M	1,2-butanediol
P-P	Cobalt palmitate “P4”	anhydrous $RuCl_3$	Sodium palmitate 0.16 M	1,2-propanediol
H-R	Cobalt heptanoate	$RuCl_3{\cdot}xH_2O$	Sodium hydroxide 0.075 M	1,2-butanediol
O-R	Cobalt octanoate	$RuCl_3{\cdot}xH_2O$	Sodium hydroxide 0.075 M	1,2-butanediol
D-R	Cobalt decanoate	$RuCl_3{\cdot}xH_2O$	Sodium hydroxide 0.075 M	1,2-butanediol

2. Physico-chemical characterization of Co particles

2.1. TEM analyses



O-R: d_{TEM} = 26 nm; L_{TEM} = 135 nm

D-R: d_{TEM} = 24 nm; L_{TEM} = 187 nm

L-R-1: d_{TEM} = 19 nm; L_{TEM} = 175 nm

L-R-2: d_{TEM} = 21 nm; L_{TEM} = 140 nm

L-R-3: d_{TEM} = 15 nm; L_{TEM} = 51 nm

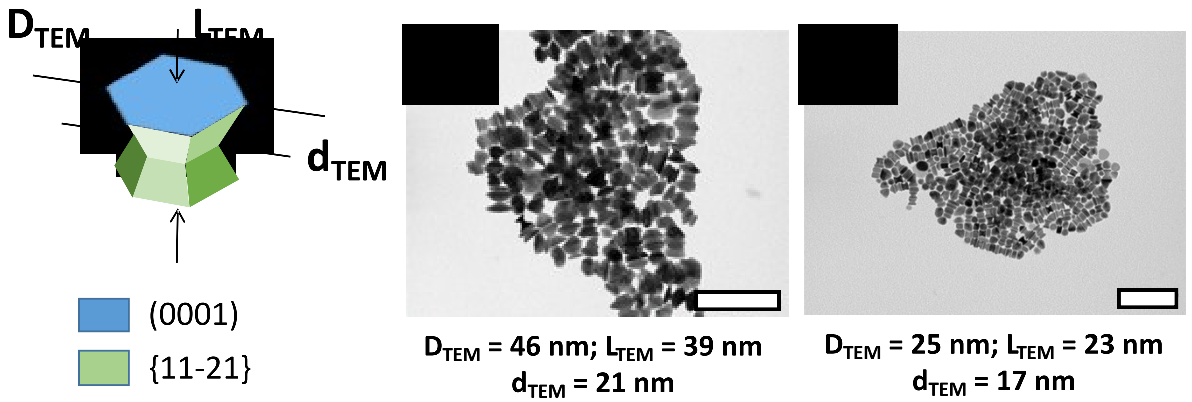
L-R-4: d_{TEM} = 14 nm; L_{TEM} = 105 nm

P-R-1: d_{TEM} = 16 nm; L_{TEM} = 80 nm

P-R-2: d_{TEM} = 20 nm; L_{TEM} = 170 nm

P-R-3: d_{TEM} = 13 nm; L_{TEM} = 35 nm

Figure S1. TEM images and mean dimensions of Co nanorods. The scale bar stands for 200 nm. L_{TEM} - mean length, d_{TEM} - mean diameter of the rods.

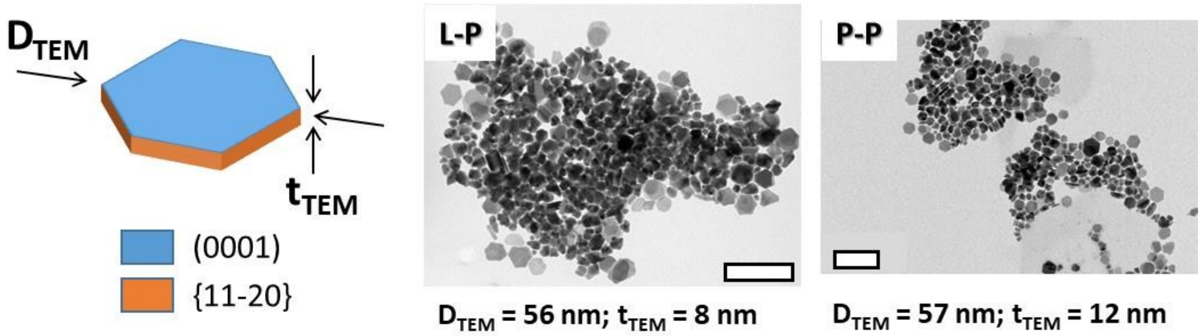


[redacted] [redacted] [redacted]

D_{TEM} = 46 nm; L_{TEM} = 39 nm d_{TEM} = 21 nm

D_{TEM} = 25 nm; L_{TEM} = 23 nm d_{TEM} = 17 nm

Figure S2. TEM images and mean dimensions of Co nanodiabolos. The scale bar stands for 200 nm. L_{TEM} - mean length; D_{TEM} - mean diameter of the diabolos tips, d_{TEM} - mean diameter of the central column in the diabolos.



D_{TEM} = 56 nm; t_{TEM} = 8 nm

D_{TEM} = 57 nm; t_{TEM} = 12 nm

Figure S3. TEM images and mean dimensions of Co nanoplatelets. The scale bar stands for 200 nm. D_{TEM} - mean diameter of the platelets, t_{TEM} - mean thickness of the platelets.

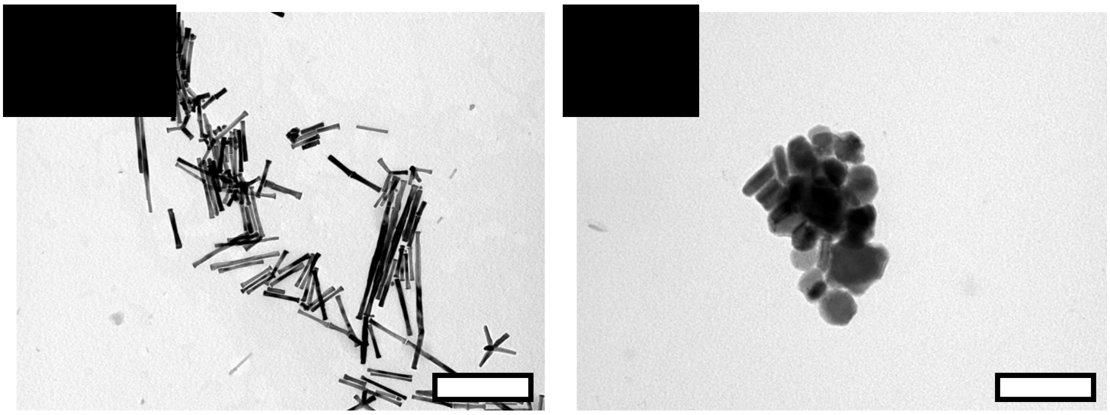


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Figure S4. TEM images of P-R-2 and P-P samples after additional washing with methanol during the synthesis. The scale bar stands for 200 nm.

2.2. X-Ray diffraction

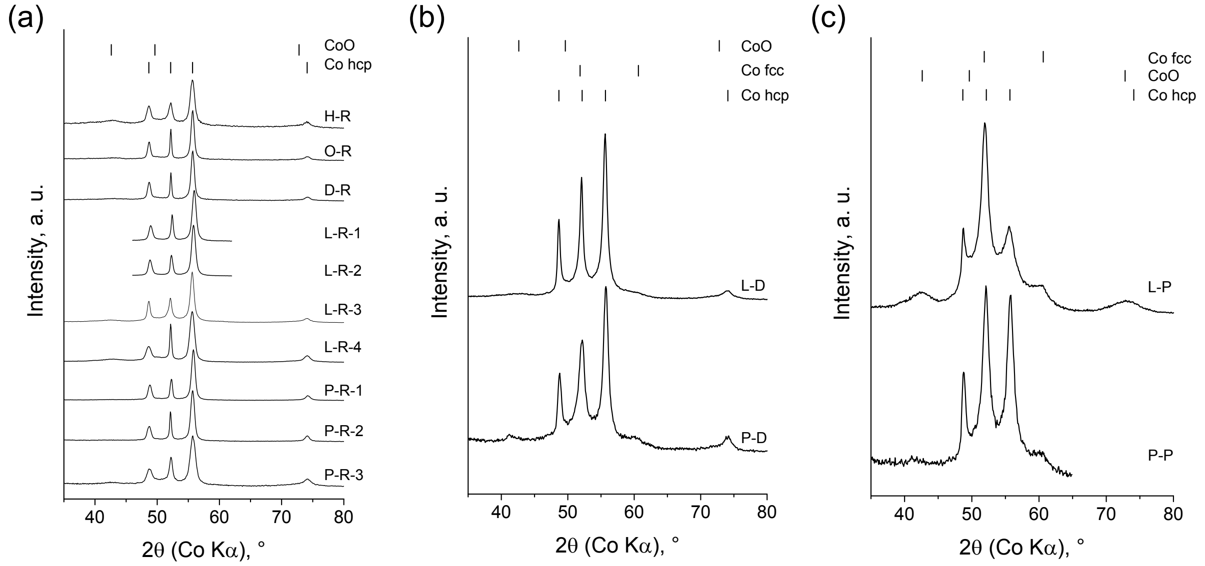

Figure S5. X-ray diffraction patterns of Co (a) nanorods, (b) diabolos and (c) platelets.

2.3. Evaluation of the expected specific surface area.

The specific surface area, SSA_C, can be calculated using the following formula:

$$SSA_C = \frac{S_{tot}}{m} = \frac{S_{tot}}{d_{Co}V}$$

with d_{Co} the density of Co (8.86 g cm^{-3}), V the volume of a NR and S_{tot} the surface area of a NR. V and S_{tot} can be calculated, as explained below.

Nanorods

$$S_{tot} = 2S_{base} + S_{lateral} = 3\sqrt{3}\left(\frac{d_{TEM}}{2}\right)^2 + 6 \times L_{TEM} \times \frac{d_{TEM}}{2}$$

$$V = S_{base} \times L_{TEM}$$

And $$V = \frac{3\sqrt{3}}{8} \times {d_{TEM}}^2 \times L_{TEM}$$

Where:

S_{base} – surface area of the base of nanoparticle

$S_{lateral}$ – surface area of the lateral facets of nanoparticle

Nanoplatelets

$$S_{tot} = 2S_{base} + S_{lateral} = 3\sqrt{3}\left(\frac{D_{TEM}}{2}\right)^2 + 6 \times t_{TEM} \times \frac{D_{TEM}}{2}$$

$$V = S_{base} \times t_{TEM}$$

And $$V = \frac{3\sqrt{3}}{8} \times D_{TEM}{}^{2} \times t_{TEM}$$

Nanodiabolos

$$S_{tot} = 2S_{base} + S_{lateral} = 3\sqrt{3}\left(\frac{D_{TEM}}{2}\right)^2 + 6 \times \left(\frac{D_{TEM}}{2} + \frac{d_{TEM}}{2}\right) \times \sqrt{L_{TEM}{}^{2} + \frac{3}{4}\left(\frac{D_{TEM}}{2} - \frac{d_{TEM}}{2}\right)^2}$$

$$V = \sqrt{3}L_{TEM} + \left(\left(\frac{D_{TEM}}{2}\right)^2 + \left(\frac{d_{TEM}}{2}\right)^2 + \left(\frac{D_{TEM}}{2} \times \frac{d_{TEM}}{2}\right)\right)$$

2.4. Thermogravimetric and differential thermal analyses.

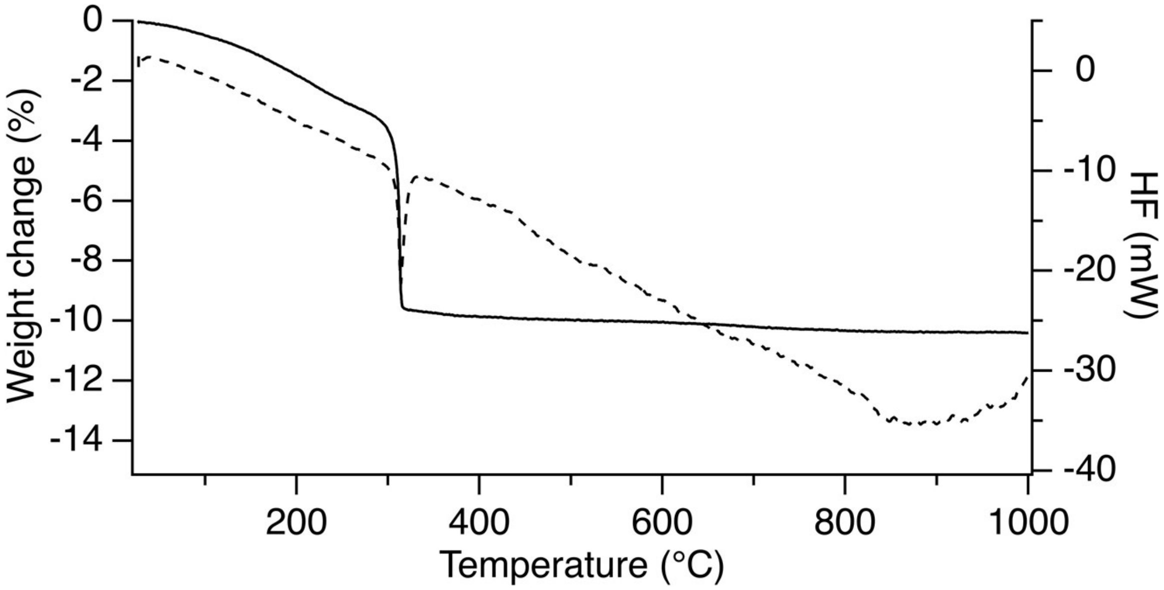

Figure S6. TGA-N_2 results analysis for L-R-1 sample. By solid line the weight change is given and by dashed line the heat flow is indicated.

3. Reactivity

Table S1. Data used to compute the TON values for the 2-octanol dehydrogenation reaction using decorated Co nanoparticles.

Sample[1]	$n_{converted\ substrate}$ (mol)	SA[2] (m^2)	Exposed facets			$n_{surface\ Co\ atoms}$[3] (10^{-6} mol)	TON[4] ($mol_{alcohol}\ mol_{surface\ Co}^{-1}$)
			(0001) (%)	(11-20) (%)	(11-21) (%)		
L-R-1	0.01529	0.67	5	95	0	13.40	1140
L-R-2	0.01393	0.59	6	94	0	11.86	1170
L-R-3	0.00148	0.71	35	20	45	22.52	70
L-R-4	0.01469	0.89	6	94	0	17.77	830
L-D	0.01307	0.61	38	0	62	21.40	610
L-P	0.01414	0.82	78	22	0	23.58	600
P-R-1	0.00071	0.41	5	95	0	8.10	90
P-R-2	0.00120	0.60	8	92	0	12.20	100
P-R-3	0.00349	0.47	14	86	0	9.96	350
P-D	0.00096	0.37	35	0	65	12.92	70
P-P	0.00473	0.40	67	33	0	11.08	430
H-R	0.00866	-	-	-	-	-	-
O-R	0.00945	0.52	8	92	0	10.61	890
D-R	0.01052	0.54	5	95	0	10.82	970

[1] Sample naming according to the role: type of ligand – shape – order number (if needed)

[2] SA – surface area exposed by Co in the catalyst sample used for the catalytic test: SA = $SSA_C \times m_{Co}$ with SSA_C the specific surface area calculated based on TEM geometric measurements and $m_{Co} = m_{cat} \times \frac{100\% - \Delta m_{TGA - N_2}}{100\%}$ ($\Delta m_{TGA - N_2}$ can be found in Table 1, in the main paper)

[3]the amount of Co atoms (mol) was calculated using the following formula: $n_{surface\ Co\ atoms} = SA \times \left\{ \left(\frac{\%(0001)}{100} \cdot \delta_{Co(0001)} \right) + \left(\frac{\%(11-20)}{100} \cdot \delta_{Co(11-20)} \right) + \left(\frac{\%(11-21)}{100} \cdot \delta_{Co(11-21)} \right) \right\}$, with $\delta_{Co(0001)}$ = 31.42 $\cdot$ 10^{-6} mol Co.m^{-2}, $\delta_{Co(11-20)}$ = 19.35 $\cdot$ 10^{-6} mol Co.m^{-2}, $\delta_{Co(11-21)}$ = 37.23 $\cdot$ 10^{-6} mol Co m^{-2}

[4]TON values accuracy ± 25 mol/mol

For example, for sample L-R-1

$$TON = \frac{n_{converted\ substrate}}{n_{surface\ Co\ atoms}}$$

$$n_{converted\ substrate} = 0.01529\ mol$$

$$n_{surface\ Co\ atoms} = SA \times \left\{ \left(\frac{\%(0001)}{100} \cdot \delta_{Co(0001)} \right) + \left(\frac{\%(11-20)}{100} \cdot \delta_{Co(11-20)} \right) + \left(\frac{\%(11-21)}{100} \cdot \delta_{Co(11-21)} \right) \right\}$$

$$SA = SSA_C \times m_{Co}$$

$$m_{Co} = m_{cat} \times \frac{100\% - \Delta m_{TGA-N_2}}{100\%}$$

$$m_{Co} = 0.0257g \cdot \left(\frac{(100-10.4)}{100} \right) = 0.0230g$$

$$SA = 29\frac{m^2}{g} \cdot 0.0230g = 0.67m^2$$

$$n_{surface\ Co\ atoms} = 0.67m^2 \times \left\{ \left(\frac{5}{100} \cdot 31.42 \cdot 10^{-6}\frac{mol}{m^2} \right) + \left(\frac{95}{100} \cdot 19.35 \cdot 10^{-6}\frac{mol}{m^2} \right) + \left(\frac{0}{100} \cdot 37.23 \cdot 10^{-6}\frac{mol}{m^2} \right) \right\} = 13.36 \cdot 10^{-6} mol$$

$$TON = \frac{0.01529\ mol}{13.36 \cdot 10^{-6} mol} \cong 1150\frac{mol}{mol}$$

Table S2. ICP-OES analysis for the solutions collected after 24 h of reaction.

Sample	C_{Co} (mg/l)	Co[#] (wt%)	Presence of precipitate*
L-R-1	<0.2	---	No
L-R-3	0.4	0.11	Yes
P-R-1	1.1	0.29	Yes
P-R-2	4.3	1.29	Yes
P-R-3	1.5	0.67	Yes
D-P	4.4	2.10	Yes
P-P	2.7	0.84	Yes

* After the reaction, solutions were filtered (0.45 μm pores filters) and put into refrigerator. After few weeks, precipitates from the reaction solutions, which probably contain cobalt, were observed. As only the supernatants from them were used in ICP-OES analysis, thus, the established concentrations of Co are only qualitative.

[#] wt% of Co leached in the solution in respect to the initial mass of Co in the catalyst

4. DFT computations

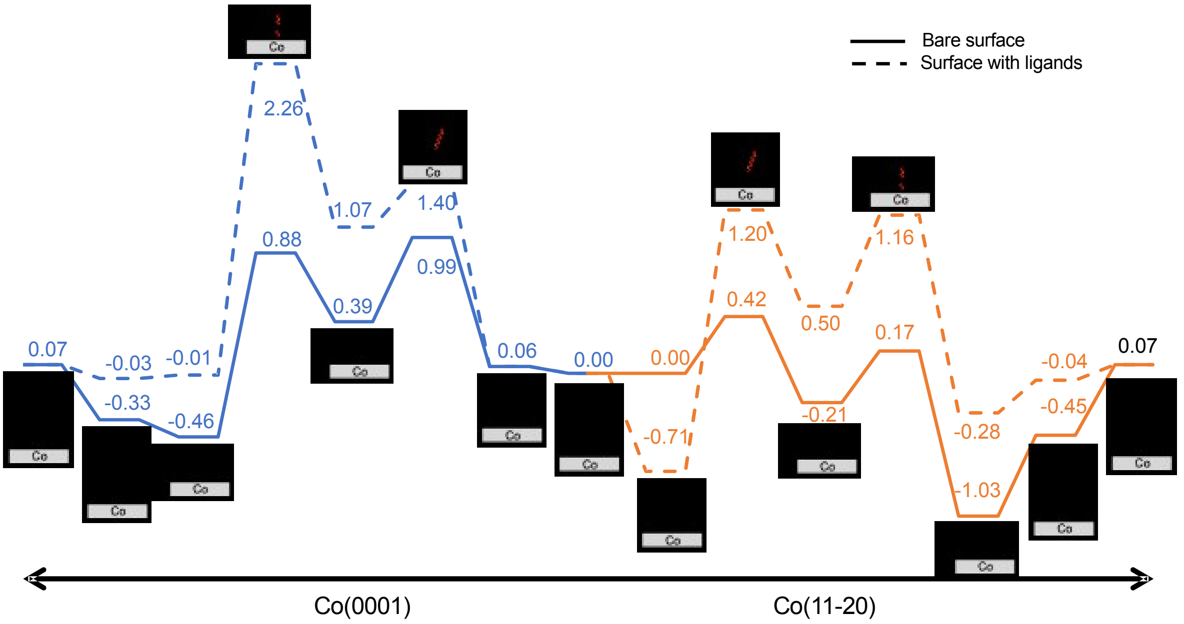

Figure S7. Gibbs Free Energy profiles for the iPrOH dehydrogenation via the hydroxyalkyl pathway on the Co(0001) facet (to the left side) and on the Co(11-20) facet (to the right side). Profiles with a solid line correspond to bare surfaces, dashed line to surface decorated with CH_3COO ligands (0.75A-Co(11-20) and 0.44A-Co(0001)). Energies are given in eV. Schematic drawings represent route stages.

Table S3. Energy spans (in eV) and activation energies (in eV) for the iPrOH dehydrogenation reaction proceeding via alkoxy or hydroxyalkyl pathways on the bare and ligand covered surfaces.

	Co(0001)	**0.44A-Co(0001)**	**Co(11-20)**	**0.75A-Co(11-20)**
		Energy span (eV)		
Alkoxy	1.49	1.24	1.13	0.99
Hydroxyalkyl	1.45	2.29	1.45	1.91
		E_{act} (eV)		
OH	0.70	0.90	0.10	0.65
OH-CH	0.62	1.05	0.48	0.99
CH	0.93	1.34	0.42	1.91
CH-OH	0.49	1.19	0.38	0.66

Table S4. Analysis of the impact of the ligands on the stability of surface species along the alkoxy path on 0.44A-Co(0001) and 0.75A-Co(11-20). All the energies are given in eV.

Surface	Surface species	$\Delta\Delta G_{ads}$ (eV)	$\Delta G_{surf\ species}$ (eV)	$\Delta G_{ligands}$ (eV)	ΔG_{slab} (eV)	$\Delta G_{deformations}$ (eV)	$\Delta G_{interactions}$ (eV)
0.44A-Co(0001)	iPrOH	0.00	0.41	0.48	0.12	0.77	-0.77
	TS-OH	0.20	0.23	0.44	0.09	0.58	-0.38
	iPrO	0.30	0.24	0.49	0.05	0.68	-0.38
	H	0.15	0.04	0.19	0.00	0.23	-0.08
	TS OH-CH	0.73	0.28	0.79	0.12	0.95	-0.22
	Acetone	0.1	0.55	0.47	0.08	0.94	-0.79
0.75A-Co(11-20)	iPrOH	-0.71	0.15	0.04	0.04	0.15	-0.86
	TS-OH	-0.16	0.29	0.12	0.16	0.25	-0.41
	iPrO	-0.09	0.15	0.15	0.05	0.25	-0.34
	H	0.20	0.12	0.08	0.08	0.12	0.08
	TS OH-CH	0.41	0.58	0.43	0.15	0.86	-0.45
	Acetone	0.35	0.53	0.08	0.09	0.52	-0.17

$\Delta\Delta G_{ads} = \Delta G_{ads-LS} - \Delta G_{ads-BS} = \Delta G_{deformations} + \Delta G_{interactions} = \Delta G_{surf\ species} + \Delta G_{ligands} - \Delta G_{slab} + \Delta G_{interactions}$

$\Delta\Delta G_{ads}$ – adsorption energy difference between a surface species adsorbed on the bare surface (BS) and the same surface species adsorbed on the same surface but covered with ligands (LS)

ΔG_{ads-LS} – adsorption energy of the surface species on the surface with ligands

ΔG_{ads-BS} - adsorption energy of the surface species on the bare surface

$\Delta G_{surf\ species}$ – change of Gibbs free energy for the surface species only in its adsorption geometry between its state on BS and the one on LS

$\Delta G_{ligands}$ – change of Gibbs free energy for the ligands only between the state without and with co-adsorbed molecule

ΔG_{slab} – change of Gibbs free energy for slab only between BS and LS

$\Delta G_{interactions}$ – change of Gibbs free energy of interactions between reactant molecule and ligands, between BS and LS